

Some Verification Problems with Possible Transport Applications

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Introduction

Verification is an essential part of the process whereby a code developer builds a sense of correctness and reliability in the answers his code produces. Unfortunately, many codes lack the machinery to make use of the method of manufactured solutions [KS03] and so are reliant for verification on problems which possess analytic solutions. The authors present here three problems they derived for their own verification purposes. We hope they may be useful to others in their search for computational correctness.

1 Open Radiation Boundary Test

This problem is meant to test the correctness of implementation for open radiation diffusion boundary conditions. It is a pure radiation diffusion flow problem with no hydrodynamics or material coupling. The solution is exact and simple to compute. Although it does require an iterative root solve, the iteration is easy to perform and generally quick to converge. Consider a 1-D slab geometry. The slabs are infinite in extent in the y and z directions. On the left is a closed radiation boundary at x=0. On the right is an open boundary at x=L. Outside the open boundary there is an incident radiative flux at temperature T_{out} . The radiation temperature inside the problem is initially at T_{in} . The Rosseland opacity k_{ross} and the density ρ are constants. The speed of light is c. The Planck opacity is zero. There is no flux limiter. Then the 1-D radiation diffusion equation is

$$\frac{\partial \phi}{\partial t} - D \frac{\partial^2 \phi}{\partial x^2} = 0 \tag{1}$$

where $D = \frac{c}{3\rho\kappa_{ross}}$ is the constant diffusion coefficient. Here $\phi = T^4$. We seek a general

time and space dependent solution for $\phi(x,t)$. If we define $\phi_{in} = T_{in}^4$ and $\phi_{out} = T_{out}^4$ then the boundary and initial conditions are

$$\phi(x,t=0) = \phi_{in}$$

$$\frac{\partial \phi(x=0,t)}{\partial x} = 0$$

$$\phi(x=L,t) + \frac{D}{2c} \frac{\partial \phi(x=L,t)}{\partial x} = \phi_{out}$$
(2)

We begin by taking the Laplace transform of Eqs. 1 and 2 getting

$$s\phi(x,s) - \phi_{in} - D\frac{\partial^2 \phi(x,s)}{\partial x^2} = 0$$
(3)

$$\frac{\partial \phi(0,s)}{\partial x} = 0 \tag{4}$$

and

$$\phi(L,s) + \frac{D}{2c} \frac{\partial \phi(L,s)}{\partial x} = \frac{\phi_{out}}{s}$$
 (5)

where s is now the Laplace transformed time variable. The general solution to Eq. 3 is

$$\phi(x,s) = A \exp(\beta x) + B \exp(-\beta x) + \frac{\phi_{in}}{s}$$
 (6)

where A and B are as yet unknown functions of s and β is defined as

$$\beta = \sqrt{\frac{s}{D}} \,. \tag{7}$$

If we apply the boundary condition at x=0 we get A=B so that Eq. 6 becomes

$$\phi(x,s) = A[\exp(\beta x) + \exp(-\beta x)] + \frac{\phi_{in}}{s}.$$
 (8)

Applying the boundary condition at x=L we have that

$$A = \frac{-(\phi_{in} - \phi_{out})}{2s[\cosh(\beta L) + (\frac{2D}{c})\beta \sinh(\beta L)]}$$
(9)

so that

$$\phi(x,s) = \frac{\phi_{in}}{s} - \frac{(\phi_{in} - \phi_{out})}{s} \frac{\cosh(\beta x)}{\left[\cosh(\beta L) + (2D/c)\beta \sinh(\beta L)\right]}.$$
 (10)

To obtain our final solution we must compute the Laplace inversion of Eq. 10. We accomplish this by directly computing the Bromwich Inversion integral

$$\phi(x,t) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} \{ \frac{\phi_{in}}{s} - \frac{(\phi_{in} - \phi_{out})\cosh(x\sqrt{s/D})}{s[\cosh(L\sqrt{s/D}) + (2/c)\sqrt{sD}\sinh(L\sqrt{s/D})]} \} e^{st} ds .$$
 (11)

This at first appears daunting but may be done exactly using the residue theorem. A branch cut is taken along the positive real axis and the integrals along the branch cut cancel. There is a simple pole at s=0 and an infinite number of simple poles at $s=-R_n$ where the R_n are the roots of

$$\cos(L\sqrt{\frac{R_n}{D}}) - \frac{2\sqrt{DR_n}}{c}\sin(L\sqrt{\frac{R_n}{D}}) = 0.$$
 (12)

This expression can be rewritten as a fixed point iteration to obtain the values of R_n as

$$R_n^{new} = \frac{D}{L^2} \left[n\pi + \arctan\left(\frac{c}{2\sqrt{DR_n^{old}}}\right) \right]^2.$$
 (13)

With an initial guess of 1.0, Eq. 13 will rapidly converge to the nth root of Eq. 12. The final solution we seek is just the sum over the residues resulting in

$$\phi(x,t) = \phi_{out} + (\phi_{in} - \phi_{out}) \sum_{n=1}^{\infty} \frac{2 \exp(-R_n t)}{\left[1 + \frac{Lc}{2D} + \frac{2LR_n}{c}\right]} \frac{\cos(x\sqrt{\frac{R_n}{D}})}{\cos(L\sqrt{\frac{R_n}{D}})}.$$
(14)

If the value of $T_{out} > T_{in}$, then a heat wave will propagate from right to left at a rate given by Eq. 14 and reach a steady state $T=T_{out}$. Likewise, if $T_{in}>T_{out}$ then a cooling wave will propagate from right to left and reach steady state $T=T_{out}$.

This test problem bears similarities to the excellent radiation diffusion test problem from Su and Olson [SO96]. But while the solution presented here is not as intricate as Su-Olson and includes less physics, it is much easier to evaluate. If one were interested in testing the boundary conditions in isolation from the other physics this problem would be a better choice.

2 Spherical Heat Flow Test

What follows is the derivation of an analytic solution for a pure heat conduction problem which should be useful for verification purposes. Consider a sphere of radius R at a constant temperature T_0 . We seek a solution to the homogeneous heat diffusion equation in spherical coordinates (exterior to the hot sphere)

$$\rho C \frac{\partial T}{\partial t} - \frac{1}{r^2} \frac{\partial}{\partial r} (\kappa r^2 \frac{\partial T}{\partial r}) = 0$$
 [15]

subject to the initial and boundary conditions

$$T(t=0,r>R) = 0$$

$$T(t,r \le R) = T_0 . [16]$$

$$T(t,r=\infty) = 0$$

In Eq.15, C is the specific heat, ρ is the density, and κ is the conduction coefficient. Specify temperature dependent forms for the specific heat and conduction coefficients as

$$\kappa = \kappa_0 T^n
C = C_0 T^n$$
[17]

where κ_0 and C_0 are constants and n is some exponent not necessarily an integer. If we substitute Eq.17 into Eq.15 and define

$$\Phi = T^{n+1} \tag{18}$$

we have

$$\rho C_0 \frac{\partial \Phi}{\partial t} - \frac{1}{r^2} \frac{\partial}{\partial r} (\kappa_0 r^2 \frac{\partial \Phi}{\partial r}) = 0.$$
 [19]

Take the Laplace transform of Eq.19 to get

$$\frac{\partial}{\partial r} \left(r^2 \frac{\partial \Phi(s, r)}{\partial r}\right) - r^2 s \frac{\rho C_0}{\kappa_0} \Phi(s, r) = 0.$$
 [20]

Now the transformed boundary conditions are

$$\Phi(s, r = R) = \frac{\Phi_0}{s} = \frac{T_0^{n+1}}{s} .$$

$$\Phi(s, r = \infty) = 0$$
[21]

This ODE has the solution (for r>R)

$$\Phi(s,r) = \frac{\Phi_0 R}{sr} \exp\{-(r-R)\sqrt{\frac{s\rho C_0}{\kappa_0}}\} .$$
 [22]

Perform the Laplace inversion to get

$$T(t,r) = \begin{cases} T_0 \\ T_0 \left[\frac{R}{r} Erfc\left\{ \frac{(r-R)}{2} \sqrt{\frac{\rho C_0}{\kappa_0 t}} \right\} \right]^{\left(\frac{1}{n+1}\right)} \end{cases} \quad \text{for} \quad r \le R \\ r > R$$
 [23]

For n = 0 this is an easy computational problem. But at large n it will strain the diffusion codes ability to accurately resolve the gradients in the material properties. This is mainly an issue because the diffusion coefficient is not a constant but will vary in space and time. Approximations or averaging schemes used in the construction of the diffusion matrix will be sorely tested for large n and typically will require a finer mesh for accurate answers. This problem was specifically constructed to test the heat conduction in a spherical geometry and in isolation from other physics in response to difficulties running another verification problem - the Coggeshall problem number 8 [Co91].

3 Coupled Multi-Temperature Diffusion Test

This is a modification of the problem in Sec. 2 meant to exercise more of the diffusion code as well as the code coupling the radiation and matter temperatures. It has radiation diffusion as well at electron and ion conduction. It is a 1-D slab geometry infinite in extent in the y and z directions. On the left at $x=x_0$ the radiation and material temperatures are fixed at T_0 . On the right boundary the problem extends to x=infinity. Hydrodynamics is turned off and there is no flux limiter on the radiation diffusion or the matter conduction. The density ρ and the radiation diffusion coefficient D are constants. The radiation and material temperature update equations are

$$\sigma \frac{\partial T_{rad}^{4}}{\partial t} - \sigma D \frac{\partial^{2} T_{rad}^{4}}{\partial x^{2}} = c \rho \sigma \kappa_{P} (T_{mat}^{4} - T_{rad}^{4})$$
(24)

$$\rho C_{ve} \frac{\partial T_{mat}}{\partial t} - \frac{\partial}{\partial x} (K_e \frac{\partial T_{mat}}{\partial x}) = c\rho \sigma \kappa_P (T_{rad}^4 - T_{mat}^4) + k_{ie} (T_{ion} - T_{mat})$$
(25)

$$\rho C_{vi} \frac{\partial T_{ion}}{\partial t} - \frac{\partial}{\partial x} (K_i \frac{\partial T_{iont}}{\partial x}) = k_{ie} (T_{mat} - T_{ion})$$
(26)

where c is the speed of light, k_{ie} is the electron-ion coupling rate, σ the radiation constant, K_e and K_i are conduction coefficients, C_{ve} and C_{vi} are specific heats, κ_p is the Planck opacity. The boundary and initial conditions are

$$T_{mat}(x = x_0, t) = T_{rad}(x = x_0, t) = T_{ion}(x = x_0, t) = T_0$$

$$T_{mat}(x = \infty, t) = T_{rad}(x = \infty, t) = T_{ion}(x = \infty, t) = 0$$

$$T_{mat}(x > x_0, t = 0) = T_{rad}(x > x_0, t = 0) = T_{ion}(x > x_0, t = 0) = 0$$
(27)

We now impose that

$$K_{e} = K_{e0} T_{mat}^{4}$$

$$K_{i} = K_{i0} T_{ion}^{4}$$
(28)

and

$$C_{ve} = C_e T_{mat}^4$$

$$C_{vi} = C_i T_{ion}^4$$
(29)

where K_{e0} , K_{i0} , C_e , C_i , are constants. We also impose $\kappa_P = k_{ie} = \infty$. This guarantees $T_{mat} = T_{rad} = T_{ion}$. We can now combine Eqs. 28 and 29 with Eqs. 24-26 to get

$$(4\sigma + \rho(C_e + C_i))\frac{\partial \phi}{\partial t} - (4\sigma D + K_{e0} + K_{i0})\frac{\partial^2 \phi}{\partial x^2} = 0$$
(30)

with

$$\phi = T^4. \tag{31}$$

The diffusion of energy can be split between the ion conduction, electron conduction and radiation diffusion to whatever extent we wish by simply modifying the coefficients. The radiation and material temperatures are locked together and we can solve Eq. 30 to get the time and space dependence of ϕ . Take the Laplace transform of Eqs. 27 and 30 to get

$$\phi(x,s)(4\sigma + \rho(C_e + C_i))s - (4\sigma D + K_{i0} + K_{e0})\frac{\partial^2 \phi(x,s)}{\partial x^2} = 0$$
(32)

and

$$\phi(x = x_0, t) = \frac{\phi_0}{s} = \frac{T_0^4}{s}.$$

$$\phi(x = \infty, t) = 0$$
(33)

This has the solution

$$\phi(x,s) = \frac{\phi_0}{s} \exp\{-\frac{1}{2}(x - x_0)\sqrt{s}\sqrt{\frac{4\sigma + \rho(C_e + C_i)}{4\sigma D + K_{e0} + K_{i0}}}\}$$
 (34)

Now we do the Laplace inversion of Eq. 34 to get

$$T(x,t) = \begin{cases} T_0 \\ T_0 Erfc \{ \frac{(x-x_0)}{2\sqrt{t}} \sqrt{\frac{4\sigma + \rho(C_e + C_i)}{4\sigma D + K_{e0} + K_{i0}}} \}^{1/4} \end{cases}$$
 for $x \le x_0$ (33)

One should be careful not to dismiss this problem as trivial just because the radiation and matter have the same temperature. This is simply part of the solution. In order to get the answer correct one must compute the ion conduction, electron conduction, radiation diffusion and the matter-to-radiation coupling correctly. An error in any one of these places will give an incorrect result.

4 Conclusion

While the body of verification problems in the literature is growing, it is still far smaller than the authors would like. And while the problems presented here are not terribly complicated, nor are they trivial. Also they are exact, easy to compute, and easy to implement. And from simple to sophisticated there is a role to play for all verification problems. Should a code fail on the more complicated verification solutions the simpler ones may provide a way of isolating what is causing the problem. And with every exact solution a computer code computes our confidence in the unverifiable solutions grows. The verification solutions presented above have proven useful to the authors and we hope others will find them so as well.

5 References

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